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# TRANSMITTAL FORM

*(to be used for all correspondence after initial filing)*

| | |
|---|---|
| Patent Number | 6,834,239 B2 |
| Issue Date | December 21, 2004 |
| First Named Inventor | Victor S. Lobanov |
| Art Unit | 1631 |
| Examiner Name | Channing Mahatan |
| Total Number of Pages in This Submission: 13 | Attorney Docket Number: 30923-709.201 |

**ENCLOSURES** *(Check all that apply)*

- ☐ Fee Transmittal Form
  - ☐ Fee Attached
- ☐ Amendment/Reply
  - ☐ After Final
  - ☐ Affidavits/declaration(s)
- ☐ Extension of Time Request
- ☐ Express Abandonment Request
- ☐ Information Disclosure Statement
- ☐ Certified Copy of Priority Document(s)
- ☐ Response to Missing Parts/ Incomplete Application
  - ☐ Response to Missing Parts under 37 CFR 1.52 or 1.53
- ☐ Drawing(s)
- ☐ Licensing-related Papers
- ☐ Petition
- ☐ Petition to Convert to a Provisional Application
- ☐ Power of Attorney, Revocation Change of Correspondence Address
- ☐ Terminal Disclaimer
- ☐ Request for Refund
- ☐ CD, Number of CD(s)
- ☐ After Allowance communication to Technology Center (TC)
- ☐ Appeal Communication to Board of Appeals and Interferences
- ☐ Appeal Communication to TC **(Appeal Notice, Brief, Reply Brief)**
- ☐ Proprietary Information
- ☐ Status Letter
- ☒ Other Enclosure(s) (please identify below):
  - Request for Certificate of Correction
  - Copy of Original Claims as Filed
  - Certificate of Correction – in duplicate
  - Itemized Return postcard

Remarks

Certificate
MAR 1 0 2005
of Correction

**SIGNATURE OF APPLICANT, ATTORNEY OR AGENT**

| | |
|---|---|
| Firm or Individual name | Tobey M. Tam, Reg. No. 54,484, WILSON SONSINI GOODRICH & ROSATI |
| Signature | |
| Date | March 3, 2005 |

**CERTIFICATE OF TRANSMISSION/MAILING**

I hereby certify that this correspondence is being facsimile transmitted to the USPTO or deposited with the United States Postal Service with sufficient postage as Express mail (Label No. EV 517726042 US in an envelope addressed to: Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450 on the date shown below.

| | | | |
|---|---|---|---|
| Typed or printed name | Michael Boyd | | |
| Signature | | Date | March 3, 2005 |

This collection of information is required by 37 CFR 1.5. The information is required to obtain or retain a benefit by the public which is to file (and by the USPTO to process) an application. Confidentiality is governed by 35 U.S.C. 122 and 37 CFR 1.14. This collection is estimated to take 2 hours to complete, including gathering, preparing, and submitting the completed application form to the USPTO. Time will vary depending upon the individual case. Any comments on the amount of time you require to complete this form and/or suggestions for reducing this burden, should be sent to the Chief Information Officer, U.S. Patent and Trademark Office, U.S. Department of Commerce, P.O. Box 1450, Alexandria, VA 22313-1450. DO NOT SEND FEES OR COMPLETED FORMS TO THIS ADDRESS. **SEND TO: Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450.**

MAR 1 4 2005

EV517726042US

*WSGR Reference No. 30923-709.201*

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

| | |
|---|---|
| In re the Patent of:<br><br>Applicant: Victor S. LOBANOV et al.<br><br>Patent No.: 6,834,239 B2<br><br>Issued: December 21, 2004<br><br>Title: *Method, System, and Computer Program Product for Determining Properties of Combinatorial Library Products from Features of Library Building Blocks* | Certificate of Mailing Under C.F.R. §1.8<br><br>I hereby certify that this correspondence and all marked attachments are being deposited by Express Mail, Express Mailing Label No.: EV 517726042 US on 3-Mar-05 addressed to: Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450.<br><br>By: _____<br>Michael Boyd |

**REQUEST FOR CERTIFICATE OF CORRECTION OF PATENT FOR OFFICE MISTAKE (37 C.F.R. 1.322)**

Attn: Certificate of Corrections Branch
Commissioner for Patents
P.O. Box 1450
Alexandria, VA 22313-1450

Dear Sir/Madam:

It is respectfully requested that a Certificate of Correction be issued in U.S. Patent No. 6,834,239 for mistakes made in printing by the U.S. Patent and Trademark Office. Applicants observe a misprint of Claim 1, steps 4 and 6. Correction thereof does not involve such changes in the patent as would constitute new matter or would require re-examination. A certificate of correction showing the following changes is requested:

1. In the claims, at column 15, line 63, claim 1, "$\{x_i = a_{1t_{i1}}|a_{2t_{i2}}|a_{rt_{ir}}\}$" should read -- $\{x_i = a_{1t_{i1}}|a_{2t_{i2}}|...|a_{rt_{ir}}\}$ --.

2. In the claims, at column 16, line 8, claim 1, "their features, $a_{1t_{z1}}$, $a_{2t_{21}}$, ..., $a_{rt_{zr}}$" should read -- their features, $a_{1tz1}$, $a_{2t_{z2}}$, ..., $a_{rt_{zr}}$ --.

Attached hereto, in duplicate, is Form PTO/SB/44 (PTO-1050), with at least one copy being suitable for printing. It is requested that these forms be certified by the Commissioner, with one form being returned to the undersigned attorney.

In addition, Applicants submit a copy of the following documents as further evidence that the mistakes made in the issued patent were errors made by the U.S. patent and Trademark Office:

- Original claims filed on August 22, 2001

No fee is believed to be due in connection with this request, since the errors were on the part of the U.S. Patent and Trademark Office. Please send the Certificate to:

Vicki G. Norton
WILSON SONSISNI GOODRICH & ROSATI
650 Page Mill Road
Palo Alto, California 94304-1050

The Commissioner is authorized to charge any additional fees which may be required, including petition fees, or credit any overpayment to Deposit Account No. 23-2415.

Respectfully submitted,

WILSON SONSINI GOODRICH & ROSATI
Professional Corporation

Dated: March 3, 2005

Tobey M. Tam, Agent for Applicant
Registration No. 54,484

WHAT IS CLAIMED IS:

1. A method for determining properties of products from a combinatorial chemical library $P$ using features of their respective building blocks, the method comprising the steps of:

(1) determining at least one feature for each building block in the combinatorial library $P$, $\{a_{ijk}, i = 1,2,\ldots,r; j = 1,2,\ldots,r_i; k = 1, 2, \ldots, n_i\}$, wherein $r$ represents the number of variation sites in the combinatorial library, $r_i$ represents the number of building blocks at the $i$-th variation site, and $n_i$ represents the number of features used to characterize each building block at the $i$-th variation site;

(2) selecting a training subset of products $\{p_i, i = 1,2,\ldots,m; p_i \in P\}$ from the combinatorial library $P$;

(3) determining $q$ properties for each compound $p_i$ in the selected training subset of products, wherein $y_i = \{y_{ij}, i = 1,2,\ldots,m, j = 1,2,\ldots,q\}$ represents the determined properties of compound $p_i$, and wherein $q$ is greater or equal to one;

(4) identifying, for each product $p_i$ of the training subset of products, the corresponding building blocks $\{t_{ij}, t_{ij} = 1, 2, \ldots, r_j, j = 1, 2, \ldots, r\}$ and concatenating their features determined in step (1) into a single vector $\{x_i = a_{1t_{i1}} \mid a_{2t_{i2}} \mid \ldots \mid a_{rt_{ir}}\}$;

(5) using a supervised machine learning approach to infer a mapping function $f$ that transforms input values $x_i$ to output values $y_i$ from the input/output pairs in the training set $T = \{(x_i, y_i), i = 1,2,\ldots,m\}$;

(6) identifying, after the mapping function $f$ is determined, for a product $p_z \in P$, the corresponding building blocks $\{t_{zj}, j = 1, 2, \ldots, r\}$ and concatenating their features, $a_{1t_{z1}}, a_{2t_{z2}}, \ldots, a_{rt_{zr}}$, into a single vector $\{x_z = a_{1t_1} \mid a_{2t_2} \mid \ldots \mid a_{rt_r}\}$, and

(7) mapping $x_z \rightarrow y_z$, using the mapping function $f$ determined in step (5), wherein $y_z$ represents the properties of product $p_z$.

2. The method of claim 1, wherein step (1) comprises the step of:
using a measured value as a feature for each building block.

3. The method of claim 1, wherein step (1) comprises the step of:
using a computed value as a feature for each building block.

4. The method of claim 1, wherein step (3) comprises the step of:
using a measured value as a property for each product of the training subset.

5. The method of claim 1, wherein step (3) comprises the step of:
using a computed value as a property for each product of the training subset.

6. The method of claim 1, wherein step (5) comprises the step of:
training a multilayer perceptron.

7. The method of claim 1, wherein
at least one of the features determined in step (1) is the same as at least one of the properties determined in step (3).

8. The method of claim 1, wherein
the building blocks comprise a plurality of reagents used to construct the combinatorial library *P*.

9. The method of claim 1, wherein
the building blocks comprise a plurality of fragments of a plurality of reagents used to construct the combinatorial library *P*.

10. The method of claim 1, wherein
the building blocks comprise a plurality of modified fragments of a plurality of reagents used to construct the combinatorial library *P*.

11. The method of claim 1, wherein step (2) comprises the step of:

selecting a training subset of products at random.

12. The method of claim 1, wherein step (2) comprises the step of:

selecting a training subset of products using a combinatorial design method to cover all pairwise combinations of building blocks.

13. The method of claim 1, wherein step (2) comprises the step of:

selecting a training subset of products using a diversity metric to select a diverse subset of products.

14. A method for determining properties of combinatorial library products from features of library building blocks, the method comprising the steps of:

(1) determining at least one feature for each building block of a combinatorial library having a plurality of products;

(2) selecting a training subset of products from the plurality of products of the combinatorial library;

(3) determining at least one property for each product of the training subset of products;

(4) identifying a building block set for each product of the training subset of products;

(5) forming an input features vector for each product of the training subset of products from the building block set for each product of the training subset of products;

(6) using a supervised machine learning approach to infer a mapping function *f* that transforms the input features vector for each product of the training subset of products to the corresponding at least one property for each product of the training subset of products;

(7) identifying building block sets for a plurality of additional products of the combinatorial library;

(8) forming input features vectors for the plurality of additional products from the building block sets for the plurality of additional products; and

(9) transforming the input features vectors for the plurality of additional products using the mapping function *f* to obtain at least one estimate property for each of the plurality of additional products.

15. The method of claim 14, wherein step (1) comprises the step of:

using a measured value as a feature for each building block of the combinatorial library.

16. The method of claim 14, wherein step (1) comprises the step of:

using a computed value as a feature for each building block of the combinatorial library.

17. The method of claim 14, wherein step (3) comprises the step of:

using a measured value as a property for each product of the training subset of products.

18. The method of claim 14, wherein step (3) comprises the step of:

using a computed value as a property for each product of the training subset of products.

19. The method of claim 14, wherein step (6) comprises the step of:

training a multilayer perceptron using the input features vector and the corresponding at least one property for each product of the training subset of products.

20. The method of claim 14, wherein

at least one of the features determined in step (1) is the same as at least one of the properties determined in step (3).

21. The method of claim 14, wherein

the building blocks of the combinatorial library comprise a plurality of reagents used to construct the combinatorial library.

22. The method of claim 14, wherein

the building blocks of the combinatorial library comprise a plurality of fragments of a plurality of reagents used to construct the combinatorial library.

23. The method of claim 14, wherein

the building blocks of the combinatorial library comprise a plurality of modified fragments of a plurality of reagents used to construct the combinatorial library.

24. The method of claim 14, wherein step (2) comprises the step of:

selecting a training subset of products at random.

25. The method of claim 14, wherein step (2) comprises the step of:

selecting a training subset of products using a combinatorial design method to cover all pairwise combinations of building blocks.

26. The method of claim 14, wherein step (2) comprises the step of: selecting a training subset of products using a diversity metric to select a diverse subset of products.

27. A system for determining properties of combinatorial library products from features of library building blocks, comprising:

a module for determining at least one feature for each building block of a combinatorial library having a plurality of products;

a module for selecting a training subset of products from the plurality of products of the combinatorial library;

a module for determining at least one property for each product of the training subset of products;

a module for identifying a building block set for each product of the training subset of products;

a module for forming an input features vector for each product of the training subset of products from the building block set for each product of the training subset of products;

a module for using a supervised machine learning approach to infer a mapping function *f* that transforms the input features vector for each product of the training subset of products to the corresponding at least one property for each product of the training subset of products;

a module for identifying building block sets for a plurality of additional products of the combinatorial library;

a module for forming input features vectors for the plurality of additional products from the building block sets for the plurality of additional products; and

a module for transforming the input features vectors for the plurality of additional products using the mapping function *f* to obtain at least one estimate property for each of the plurality of additional products.

28. A system for determining properties of combinatorial library products from features of library building blocks, comprising:

means for determining at least one feature for each building block of a combinatorial library having a plurality of products;

means for selecting a training subset of products from the plurality of products of the combinatorial library;

means for determining at least one property for each product of the training subset of products;

means for identifying a building block set for each product of the training subset of products;

means for forming an input features vector for each product of the training subset of products from the building block set for each product of the training subset of products;

means for using a supervised machine learning approach to infer a mapping function *f* that transforms the input features vector for each

product of the training subset of products to the corresponding at least one property for each product of the training subset of products;

means for identifying building block sets for a plurality of additional products of the combinatorial library;

means for forming input features vectors for the plurality of additional products from the building block sets for the plurality of additional products; and

means for transforming the input features vectors for the plurality of additional products using the mapping function *f* to obtain at least one estimate property for each of the plurality of additional products.

29. A computer program product for determining properties of combinatorial library products from features of library building blocks, said computer program product comprising a computer useable medium having computer program logic recorded thereon for controlling a processor, said computer program logic comprising:

a procedure that enables said processor to determine at least one feature for each building block of a combinatorial library having a plurality of products;

a procedure that enables said processor to select a training subset of products from the plurality of products of the combinatorial library;

a procedure that enables said processor to determine at least one property for each product of the training subset of products;

a procedure that enables said processor to identify a building block set for each product of the training subset of products;

a procedure that enables said processor to form an input features vector for each product of the training subset of products from the building block set for each product of the training subset of products;

a procedure that enables said processor to use a supervised machine learning approach to infer a mapping function *f* that transforms the input features vector for each product of the training subset of products to the corresponding at least one property for each product of the training subset of products;

a procedure that enables said processor to identify building block sets for a plurality of additional products of the combinatorial library;

a procedure that enables said processor to form input features vectors for the plurality of additional products from the building block sets for the plurality of additional products; and

a procedure that enables said processor to transform the input features vectors for the plurality of additional products using the mapping function *f* to obtain at least one estimate property for each of the plurality of additional products.

30. The computer program product of claim 29, further comprising:

a procedure that enables said processor to train a multilayer perceptron using the input features vector and the corresponding at least one property for each product of the training subset of products.

31. The computer program product of claim 29, further comprising:

a procedure that enables said processor to use a measured value as a property for each product of the training subset of products.

32. The computer program product of claim 29, further comprising:

a procedure that enables said processor to use a computed value as a property for each product of the training subset of products.

33. The computer program product of claim 29, further comprising:

a procedure that enables said processor to use a measured value as a feature for each building block of the combinatorial library.

34. The computer program product of claim 29, further comprising:

a procedure that enables said processor to use a computed value as a feature for each building block of the combinatorial library.

35. The computer program product of claim 29, wherein

the building blocks of the combinatorial library comprise a plurality of reagents used to construct the combinatorial library.

36. The computer program product of claim 29, wherein

the building blocks of the combinatorial library comprise a plurality of fragments of a plurality of reagents used to construct the combinatorial library.

37. The computer program product of claim 29, wherein

the building blocks of the combinatorial library comprise a plurality of modified fragments of a plurality of reagents used to construct the combinatorial library.

38. The computer program product of claim 29, further comprising:

a procedure that enables said processor to select the training subset of products at random.

39. The computer program product of claim 29, further comprising:

a procedure that enables said processor to select the training subset of products using a combinatorial design method to cover all pairwise combinations of building blocks.

40. The computer program product of claim 29, further comprising:

a procedure that enables said processor to select the training subset of products using a diversity metric to select a diverse subset of products.

Staple Here Only Printer's Trim Line →

# UNITED STATES PATENT AND TRADEMARK OFFICE
# CERTIFICATE OF CORRECTION

PATENT NO. : 6,834,239

DATED :December 21, 2004

INVENTOR(s) :Lobanov *et al.*

It is certified that error appears in the above-identified patent and that said Letters Patent is hereby corrected as shown below:

In the claims, at column 15, line 63, claim 1:

"$\{x_i = a_{1t_{i1}}|a_{2t_{i2}}|a_{rt_{ir}}\}$" should read -- $\{x_i = a_{1t_{i1}}|a_{2t_{i2}}|...|a_{rt_{ir}}\}$ --.

In the claims, at column 16, line 8, claim 1:

"their features, $a_{1t_{z1}}$, $a_{2t_{21}}$, ..., $a_{rt_{zr}}$" should read -- their features, $a_{1tz1}$, $a_{2t_{z2}}$, ..., $a_{rt_{zr}}$ --.

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MAR 14 2005

Staple Here Only Printer's Trim Line →

# UNITED STATES PATENT AND TRADEMARK OFFICE
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MAR 14 2005